

Product Name: CL 316243 disodium salt

Catalog No.: 1499

Batch No.: 8

CAS Number: 151126-84-0

IUPAC Name: 5-[(2*R*)-2-[[[(2*R*)-2-(3-Chlorophenyl)-2-hydroxyethyl]amino]propyl]-1,3-benzodioxole-2,2-dicarboxylic acid disodium salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₁₈ClNa₂O₇·1¼H₂O

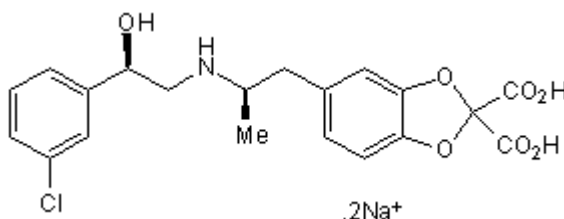
Batch Molecular Weight: 488.32

Physical Appearance: Pale yellow solid

Solubility: water to 100 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.33 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

HPLC: Shows 98.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	49.19	4.23	2.87
Found	49.15	4.32	2.92

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Description:

Potent and highly selective β_3 -adrenoceptor agonist ($EC_{50} = 3$ nM); > 10000-fold selective over β_1 and β_2 receptors. Increases brown adipose tissue thermogenesis and metabolic rate, and decreases blood insulin and glucose levels following oral administration in vivo.

Physical and Chemical Properties:

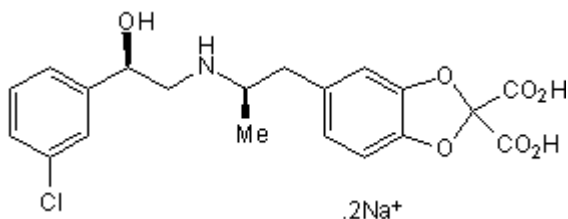
Batch Molecular Formula: $C_{20}H_{18}ClNa_2O_7 \cdot 1\frac{1}{4}H_2O$

Batch Molecular Weight: 488.32

Physical Appearance: Pale yellow solid

Minimum Purity: >96%

Batch Molecular Structure:



Storage: Desiccate at $-20^{\circ}C$

Solubility & Usage Info:

water to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a $45-60^{\circ}C$ water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Bloom et al (1992) Disodium(*R,R*)-5-[2-[[2-(3-chlorophenyl)-2-hydroxyethyl]-amino]propyl]-1,3-benzodioxole-2,2-dicarboxylate (CL 316,243). A potent β -adrenergic agonist virtually specific for β_3 receptors. A promising antidiabetic and antiobesity agent. *J.Med.Chem.* **35** 3081. PMID: 1354264.

Yoshida et al (1994) Anti-obesity and anti-diabetic effects of CL 316,243, a highly specific β_3 -adrenoceptor agonist, in yellow KK mice. *Life Sci.* **54** 491. PMID: 8309351.

Woods et al (2001) Efficacy of the β_3 -adrenergic receptor agonist CL-316243 on experimental bladder hyperflexia and detrusor instability in the rat. *J.Urol.* **166** 1142. PMID: 11490313.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956